Black box variation Bayes

"Black box variational Bayes" (BBVI) is a set of techniques for quickly and automatically approximating Bayesian posteriors using optimization. I'll consider "mean field automatic differentiation variational inference" (ADVI).

Let θ denote model parameters and y some data and the joint generating distribution be $\mathbb{P}(\theta,y) = \mathbb{P}(y|\theta)\mathbb{P}(\theta)$. Let $\mathbb{Q}(\theta|\eta)$ be a family of candidate approximate posteriors, here taken to be independent normals.

ADVI aims to find

$$\overset{*}{\eta} := \operatorname*{argmin}_{\eta} \operatorname{KL} \left(\mathbb{Q} \left(\theta | \eta \right) || \mathbb{P} \left(\theta | y \right) \right) = \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathcal{N}(z)} \left[f(z | \eta) \right]$$

for a cleverly constructed, automatically-differentiable $\eta \mapsto f(z|\eta)$.

Unfortunately, $\mathbb{E}_{\mathcal{N}(z)}[f(z|\eta)]$ is typically intractable. So ADVI uses stochastic gradient (SG). The leads to the following problems:

- You have to tune the step size carefully
- You can't assess convergence directly
- You can't compute sensitivity, so you can't use linear response covariances.

 \Rightarrow Optimization is slow and imprecise, and the posterior uncertainty is no good. Not so black box actually!

We propose a simple alternative to SG that resolves these problems (sometimes).

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where $\mathbb{P}\left(z\right)$ is known, but the expectation is not available in closed form.

2

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where $\mathbb{P}(z)$ is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where $\mathbb{P}(z)$ is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

2

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \underset{\eta}{\operatorname{argmin}} \mathbb{E}_{\mathbb{P}(z)} \left[f(z|\eta) \right] := \underset{\eta}{\operatorname{argmin}} \ell(\eta),$$

where $\mathbb{P}(z)$ is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

- Stochastic gradient (SG)
 - Update with $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$ for some step size ρ (new z_n every step)
 - · Approximately minimizes the exact objective

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where $\mathbb{P}(z)$ is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

- Stochastic gradient (SG)
 - Update with $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$ for some step size ρ (new z_n every step)
 - Approximately minimizes the exact objective
- Sample average approximation (SAA)
 - Find $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$ for fixed z_n
 - Exactly minimizes approximate objective

Suppse you want to minimize an objective function of the form

$$\mathring{\eta} := \operatorname*{argmin}_{\eta} \mathbb{E}_{\mathbb{P}(z)} \left[f(z|\eta) \right] := \operatorname*{argmin}_{\eta} \ell(\eta),$$

where $\mathbb{P}(z)$ is known, but the expectation is not available in closed form.

When does this happen?

- Black box variational inference
- Stochastic control (e.g. you have a factory, and supply and demand are random)

What can you do? There are two options, both using the Monte Carlo (MC) estimate

$$\hat{\ell}(\eta) := \frac{1}{N} \sum_{n=1}^{N} f(z_n | \eta) \approx \ell(\eta).$$

- Stochastic gradient (SG)
 - Update with $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$ for some step size ρ (new z_n every step)
 - · Approximately minimizes the exact objective
- Sample average approximation (SAA)
 - Find $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$ for fixed z_n
 - Exactly minimizes approximate objective

Which is better? In general, it depends.

As far as we can tell, the BBVI literature has only ever considered SG.

Sample average approximation (SAA)

- Find $\hat{\eta} := \operatorname{argmin}_{\eta} \hat{\ell}(\eta)$
- \bullet Fixed z_n for whole procedure
- Exactly minimizes approximate objective

Advantages:

- Can use fast off-the-shelf second-order optimization (great for poorly-conditioned problems)
- Can evaluate the objective function exactly to check for convergence
- Can compute sensitivity (linear response covariances ⇒ more accurate posterior covariances for mean field approximations)

Stochastic gradient (SG)

- $\eta^i = \eta^{i-1} \rho \nabla_{\eta} \hat{\ell}(\eta)$
- New z_n every step
- Approximately minimizes the exact objective

Advantages:

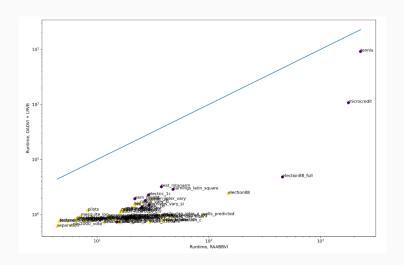
 Uses each draw z_n only once (for a single gradient step)

This is actually a big one. Because if $\eta \in \mathbb{R}^D$, in general, both SG and SAA have accuracy $(D/N)^{-1/2}$, where N is the *total* number of draws of z_n used.

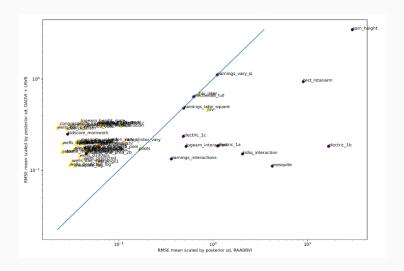
SAA uses each draw at each step of optimization. SG uses each draw once. \Rightarrow In general, SG is much more efficient in high dimensions!

Theorem (us). If $\log \mathbb{P}(\theta, y)$ is high dimensional due to a large number of "local" variables, then the accuracy is $(\log D/N)^{-1/2}$, rendering SAA feasible.

Experimental results: Runtime



Experimental results: Means



Experimental results: Standard deviations

